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THE CONSTRUCTION OF JACOBI AND PERIODIC JACOBI MATRICES WITH PR--ETC(U)

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THE CONSTRUCTION OF JACOBI AND PERIODIC
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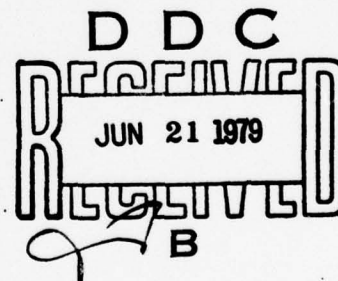
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THE CONSTRUCTION OF JACOBI AND PERIODIC JACOBI MATRICES
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Warren E. Ferguson, Jr.

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ABSTRACT

The spectral properties of Jacobi and periodic Jacobi matrices are analyzed and algorithms for the construction of Jacobi and periodic Jacobi matrices with prescribed spectra are presented. Numerical evidence demonstrates that these algorithms are of practical utility. These algorithms have been used in studies of the periodic Toda lattice, and might also be used in studies of inverse eigenvalue problems for Sturm-Liouville equations and Hill's equation.

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Jacobi matrix, periodic tridiagonal matrix,
periodic Jacobi matrix, Floquet theory,
resolvent identities.

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Significance and Explanation

In this report we present algorithms which solve two inverse eigenvalue problems that arise in matrix theory. Computational evidence is presented that demonstrates that these algorithms are of practical utility.

The first inverse eigenvalue problem considers what additional information uniquely determines the entries of a Jacobi matrix if we know its eigenvalues. Recall that a Jacobi matrix is a real, symmetric tridiagonal matrix whose next to diagonal entries are positive.

The second inverse eigenvalue problem considers what additional information uniquely determines the entries of a periodic Jacobi matrix if we know its eigenvalues. A periodic Jacobi matrix is obtained by replacing the entries in the upper right and lower left corners of a Jacobi matrix by the same positive number.

Inverse eigenvalue problems of this nature arise in mathematical physics. For example, the construction of a linear array of masses interconnected by springs with prescribed normal modes of vibration leads to such inverse eigenvalue problems. In addition, the construction of a ladder network of inductors and capacitors with prescribed transmission characteristics also leads to such inverse eigenvalue problems.

Finally, FORTRAN subroutines which implement these algorithms are presented in an appendix.

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THE CONSTRUCTION OF JACOBI AND PERIODIC JACOBI MATRICES
WITH PRESCRIBED SPECTRA

Warren E. Ferguson, Jr.

1. Introduction. A periodic Jacobi matrix is any real, symmetric matrix of the form

$$L = \begin{bmatrix} a_1 & b_1 & & & b_N \\ & b_1 & & & b_{N-1} \\ & & 0 & & \\ & & & b_{N-1} & a_N \\ b_N & & & b_{N-1} & \end{bmatrix} \quad \text{where } b_i > 0 \quad \forall i.$$

This paper shows how one can construct a periodic Jacobi matrix with prescribed spectra. For example, there is a family of periodic Jacobi matrices with $\lambda_1, \dots, \lambda_N$ as eigenvalues if and only if the numbers $\lambda_1, \dots, \lambda_N$ are real and can be ordered so that

$$\lambda_1 > \lambda_2 \geq \lambda_3 > \lambda_4 \geq \lambda_5 > \dots$$

Similar problems have been studied by other authors [2, 12].

The results presented in this paper are based upon an analysis of the spectral properties of periodic Jacobi matrices. The main tool in this analysis is the knowledge of the spectral properties of Jacobi matrices. Recall that a Jacobi matrix is any real, symmetric tridiagonal matrix whose next to diagonal entries are positive. Our canonical Jacobi matrix will be the matrix obtained by deleting from L the last row and column, that is

$$J = \begin{bmatrix} a_1 & b_1 & & & 0 \\ & b_1 & & & \\ & & & & b_{N-2} \\ & & & b_{N-2} & a_{N-1} \\ 0 & & & & \end{bmatrix} \quad \text{where } b_i > 0 \quad \forall i.$$

An algorithm which constructs a Jacobi matrix with prescribed spectra is presented in Theorem 2. This algorithm is derived from the fact that any real, symmetric matrix has real eigenvalues and a corresponding full set of real, orthonormal eigenvectors. We hasten to point out that essentially the same algorithm was presented by de Boor and Golub [3]. Similar problems have been studied by other authors [8, 9].

The spectral properties of periodic Jacobi matrices are considered in Section 3. The results presented in this section are derived from a matrix analog of Floquet theory [11]. In Section 4 we use these results to characterize the family of periodic Jacobi matrices with prescribed spectra.

We present the results of several numerical experiments in Section 5. These results demonstrate that the algorithms presented in Theorems 2 and 6 are of practical utility. Indeed, these algorithms have been used in performing numerical experiments on the periodic Toda lattice [4]. In Section 6 we conclude the paper with several comments.

2. Spectral Properties of Jacobi Matrices. In this section we will consider the spectral properties of the Jacobi matrix

$$J = \begin{bmatrix} a_1 & b_1 & & 0 \\ & \ddots & \ddots & \\ & b_1 & \ddots & b_{N-2} \\ & & & 0 & b_{N-2} & a_{N-1} \end{bmatrix} \quad \text{where } b_i > 0 \quad \forall i.$$

Observe that J is a real, symmetric matrix. Consequently J has real eigenvalues μ_1, \dots, μ_{N-1} and a corresponding set Y_1, \dots, Y_{N-1} of real, orthonormal eigenvectors [13,14]. If Y denotes the matrix whose j th column is Y_j then Y is an orthogonal matrix and

$$JY = YD \quad \text{where} \quad D = \begin{bmatrix} \mu_1 & & 0 \\ & \ddots & \\ 0 & & \mu_{N-1} \end{bmatrix}. \quad (1)$$

Many important relationships between the eigenvalues and eigenvectors of J can be derived from the representation

$$(\mu I - J)^{-1} = Y(\mu I - D)^{-1} Y^T \quad (2)$$

of the resolvent of J . For example, by comparing the entries in row 1, column $N-1$ of (2) we arrive at the identity

$$b_1 \cdots b_{N-2} = \sum_{k=1}^{N-1} \frac{\omega(\mu)}{\mu - \mu_k} Y_{1,k} Y_{N-1,k}. \quad (3.a)$$

Here

$$\omega(\mu) = \det(\mu I - J) \quad (3.b)$$

is the characteristic polynomial of J and $Y_{i,j}$ denotes the entry of Y in row i , column j . Another important identity, used by Stieltjes in his treatment of inverse eigenvalue problems, can be derived from (2) by comparing the entries in row 1, column 1 (or row $N-1$, column $N-1$.)

In the work that follows we will demonstrate that the entries of J can be recovered from the entries on the diagonal of D and in the first row of Y . Before we describe this process let us introduce the following:

Definition 1: (a) The Jacobi matrix J is characterized by the data $\{\mu, y\}$ if and only if

- (1) μ_1, \dots, μ_{N-1} are the eigenvalues of J , and
- (2) y_1, \dots, y_{N-1} are the first components of a set Y_1, \dots, Y_{N-1} of real, orthonormal eigenvectors of J corresponding to μ_1, \dots, μ_{N-1} .

(b) The data $\{\mu, y\}$ is compatible if and only if

- (1) μ_1, \dots, μ_{N-1} are real, distinct numbers, and
- (2) y_1, \dots, y_{N-1} are real, nonzero numbers whose squares sum to one.

We feel justified in using the words "characterize" and "compatible" in this manner because the following theorem is true.

Theorem 2: Data characterizing a Jacobi matrix is compatible. Furthermore each set of compatible data $\{\mu, y\}$ characterizes a unique Jacobi matrix J . The entries (a, b) of this Jacobi matrix are computed by the algorithm:

1. $y_{0,j} = 0 \quad \forall j$
2. $y_{1,j} = y_j \quad \forall j$
3. For $i = 1, \dots, N-2$
4. $a_i = \sum_{k=1}^{N-1} \mu_k y_{i,k}^2$
5. $b_i^2 = \sum_{k=1}^{N-1} [(\mu_k - a_i) y_{i,k} - b_{i-1} y_{i-1,k}]^2$
6. $y_{i+1,j} = \frac{1}{b_i} [(\mu_j - a_i) y_{i,j} - b_{i-1} y_{i-1,j}] \quad \forall j$
7. Next i
8. $a_{N-1} = \sum_{k=1}^{N-1} \mu_k y_{N-1,k}^2$

Proof: The proof of this theorem will be presented as a sequence of three lemmas. ■

Lemma 2.1: Data characterizing a Jacobi matrix is compatible.

Proof: Let the Jacobi matrix J be characterized by the data $\{\mu, y\}$. The μ 's are necessarily real because they are the eigenvalues of a real, symmetric matrix. By definition the y 's are real, and their squares sum to one because they may be considered to be the entries in the first row of the orthogonal matrix Y in (1). Consider the limiting form of the identity (3) as μ tends to μ_j . If μ_j were a repeated eigenvalue then $\omega'(\mu_j) = 0$ and so we would be forced to conclude that $b_1 \cdots b_{N-2} = 0$, which is impossible because each $b_i > 0$. Therefore the μ 's are distinct and, as μ tends to μ_j , we infer that

$$b_1 \cdots b_{N-2} = \omega'(\mu_j) Y_{1,j} Y_{N-1,j} \quad \forall j. \quad (4)$$

Consequently the y 's are nonzero because $y_j = Y_{1,j}$.

Lemma 2.2: Given compatible data $\{\mu, y\}$ the algorithm of Theorem 2 computes the entries (a, b) of a Jacobi matrix J characterized by the data $\{\mu, y\}$.

Proof: First, we infer that this algorithm computes the entries (a, b) of some Jacobi matrix J only if the value of b_i computed in step 5 is never zero. From the compatibility of the data we infer that $b_1 > 0$. If $b_1, \dots, b_{\ell-1} > 0$ but $b_\ell = 0$ for some $\ell < N-1$ then step 6 implies

$$\begin{bmatrix} a_1 & b_1 & & 0 \\ & b_1 & & \\ & & \ddots & \\ & & & b_{\ell-1} \\ 0 & & & b_{\ell-1} & a_\ell \end{bmatrix} \begin{bmatrix} Y_{1,j} \\ Y_{\ell,j} \end{bmatrix} = \mu_j \begin{bmatrix} Y_{1,j} \\ Y_{\ell,j} \end{bmatrix} \quad \forall j.$$

But this is impossible, for no matrix of order $\ell < N-1$ has $N-1$ distinct eigenvalues.

Second, we will demonstrate that the numbers $Y_{i,j}$ computed by this algorithm form the entries of an orthogonal matrix Y , that is the rows of Y satisfy the orthonormality relations

$$\sum_{k=1}^{N-1} Y_{i,k} Y_{j,k} = \delta_{i,j} \quad \text{for } j = 1, \dots, i \quad (5)$$

and $i = 1, \dots, N-1$. From the compatibility of the data $\{\mu, y\}$ we infer that (5) is true for $i = 1$. If (5) is true for $i = 1, \dots, \ell$ then the following argument demonstrates that it is also true for $i = \ell+1$. Clearly steps 5 and 6 imply that (5) is true for $j = \ell+1$. For $j \leq \ell$ step 6 implies that

$$\sum_{k=1}^{N-1} Y_{\ell+1,k} Y_{j,k} = \frac{1}{b_\ell} \left[\sum_{k=1}^{N-1} \mu_k Y_{\ell,k} Y_{j,k} - a_\ell \delta_{\ell,j} - b_{\ell-1} \delta_{\ell-1,j} \right].$$

The right side of this equality is zero for $j = l$ because step 4 was executed, and it is zero for $j < l$ because step 6 implies that

$$\sum_{k=1}^{N-1} \mu_k Y_{l,k} Y_{j,k} = \sum_{k=1}^{N-1} Y_{l,k} [b_{j-1} Y_{j-1,k} + a_j Y_{j,k} + b_j Y_{j+1,k}] = b_j \delta_{l,j+1}.$$

Third, we will demonstrate that the data $\{\mu, y\}$ characterizes J . It will be sufficient to prove that the matrices J, Y constructed by this algorithm satisfy (1). Step 6 implies that $JY = YD$ if we can show that the numbers

$$Y_{N,j} \equiv (\mu_j - a_{N-1})Y_{N-1,j} - b_{N-2}Y_{N-2,j} \quad \forall j$$

are zero. The techniques presented in the previous paragraph can be used to demonstrate that

$$\sum_{k=1}^{N-1} Y_{N,k} Y_{j,k} = 0 \quad \text{for } j = 1, \dots, N-1.$$

Since the rows of Y form a real, orthonormal basis we infer that

$$Y_{N,j} = 0 \quad \forall j$$

Lemma 2.3: Each set of compatible data characterizes at most one Jacobi matrix.

Proof: Let \hat{J} be any Jacobi matrix characterized by the compatible data $\{\mu, y\}$. Then y_1, \dots, y_{N-1} are the first components of a set $\hat{Y}_1, \dots, \hat{Y}_{N-1}$ of real, orthonormal eigenvectors of \hat{J} corresponding to the eigenvalues μ_1, \dots, μ_{N-1} . If \hat{Y} denotes the matrix whose j^{th} column is \hat{Y}_j then \hat{Y} is an orthogonal matrix and

$$\hat{J} \hat{Y} = \hat{Y} \hat{D} \quad \text{where} \quad \hat{D} = \begin{bmatrix} \mu_1 & & 0 \\ & \ddots & \\ 0 & & \mu_{N-1} \end{bmatrix}.$$

We will now prove that the entries (\hat{a}, \hat{b}) of \hat{J} are identical to the entries (a, b) of the Jacobi matrix J computed by the algorithm presented in Theorem 2.

The entries $\hat{Y}_{i,j}$ of \hat{Y} satisfy the orthonormality relations

$$\sum_{k=1}^{N-1} \hat{Y}_{i,k} \hat{Y}_{j,k} = \delta_{i,j} \quad \forall i, j$$

because $\hat{Y} \hat{Y}^T = I$. The entries $\hat{Y}_{i,j}$ of \hat{Y} also satisfy the recurrence relation

$$\hat{b}_{i-1} \hat{Y}_{i-1,j} + \hat{a}_i \hat{Y}_{i,j} + \hat{b}_i \hat{Y}_{i+1,j} = \mu_j \hat{Y}_{i,j} \quad \forall i, j$$

where

$$\hat{Y}_{0,j} = 0 \quad \text{and} \quad \hat{Y}_{N,j} = 0 \quad \forall j$$

because $\hat{J} \hat{Y} = \hat{Y} \hat{D}$. When the recurrence relation is multiplied by $\hat{Y}_{i,j}$ and the result is summed over j we find, using the orthonormality relations, that

$$\hat{a}_i = \sum_{k=1}^{N-1} \mu_k \hat{Y}_{i,k}^2.$$

The recurrence relation also implies that

$$\hat{Y}_{i+1,j} = \frac{1}{\hat{b}_i} [(\hat{u}_j - \hat{a}_i) \hat{Y}_{i,j} - \hat{b}_{i-1} \hat{Y}_{i-1,j}] \quad \forall j$$

and, when this identity is squared and the result is summed over j , the orthonormality relations imply that

$$\hat{b}_i^2 = \sum_k^{N-1} [(\hat{u}_k - \hat{a}_i) \hat{Y}_{i,k} - \hat{b}_{i-1} \hat{Y}_{i-1,k}]^2.$$

Starting with the fact that

$$\hat{Y}_{1,j} = Y_j \quad \forall j$$

it is easily shown by induction, following the sequence of computations presented in the algorithm, that the entries (\hat{a}, \hat{b}) of \hat{J} are identical to the entries (a, b) of J .

3. Spectral Properties of Periodic Jacobi Matrices. In this section we will consider the spectral properties of the periodic Jacobi matrix

$$L = \begin{bmatrix} a_1 & b_1 & & & b_N \\ & b_1 & & & \\ & & 0 & & \\ & & & b_{N-1} & \\ b_N & & 0 & b_{N-1} & a_N \end{bmatrix} \quad \text{where } b_i > 0 \quad \forall i.$$

Throughout this section we will use J to represent the Jacobi matrix obtained by deleting from L the last row and column.

Observe that L is a real, symmetric matrix. Consequently L has real eigenvalues and corresponding set of real, orthonormal eigenvectors [13, 14]. Let z be an eigenvector of L corresponding to the eigenvalue λ . Then the components z_i of z form a nontrivial solution of the recurrence relation $(b_0 \equiv b_N)$

$$b_{i-1} z_{i-1} + a_i z_i + b_i z_{i+1} = \lambda z_i \quad \forall i$$

which satisfies the boundary conditions

$$z_N = z_0 \quad \text{and} \quad z_{N+1} = z_1.$$

By analogy with Floquet theory, which analyzes the analogous problem for ordinary differential equations [11], let us consider the nontrivial solutions of the recurrence relation which satisfy the boundary conditions

$$z_N = \rho z_0 \quad \text{and} \quad z_{N+1} = \rho z_1.$$

Here the parameter ρ is called the Floquet multiplier of z . This problem has only the trivial solution when $\rho = 0$, while for $\rho \neq 0$ a nontrivial solution exists if and only if λ is an eigenvalue of the matrix

$$L_\rho = \begin{bmatrix} a_1 & b_1 & & 0 & \frac{1}{\rho} b_N \\ b_1 & & & & b_{N-1} \\ & & & & \\ & 0 & & b_{N-1} & a_N \\ \rho b_N & & & & \end{bmatrix}$$

With these facts in mind let us introduce the following:

Definition 3: Let J be characterized by the data $\{u, y\}$ and have $\omega(u)$ as its characteristic polynomial. Then the Floquet multipliers $\rho_1, \dots, \rho_{N-1}$ of L corresponding to u_1, \dots, u_{N-1} are the numbers defined by the relation

$$b_1 \cdots b_N = -\rho_j \omega'(u_j) b_N^2 y_j^2 \quad \forall j. \quad (6)$$

Theorem 4: The characteristic polynomial of L_ρ admits the representation

$$\det(\lambda I - L_\rho) = b_1 \cdots b_N \left\{ \Delta(\lambda) - \left(\rho + \frac{1}{\rho} \right) \right\} \quad (7)$$

where $\Delta(\lambda)$, called the discriminant of L , is independent of ρ . The Floquet multipliers $\rho_1, \dots, \rho_{N-1}$ of L corresponding to the eigenvalues u_1, \dots, u_{N-1} of J satisfy the relation

$$\Delta(u_j) = \rho_j + \frac{1}{\rho_j} \quad \forall j. \quad (8)$$

The eigenvalues $\lambda_1, \dots, \lambda_N$ of L are real and can be ordered so that

$$\lambda_1 > \lambda_2 > \lambda_3 > \lambda_4 > \lambda_5 > \dots$$

Proof: Using elementary properties of determinants it is not hard to demonstrate that

$$\frac{d}{d\rho} \det(\lambda I - L_\rho) = -b_1 \cdots b_N \left(1 - \frac{1}{\rho^2} \right).$$

When both sides are integrated with respect to ρ we find that

$$\det(\lambda I - L_\rho) = b_1 \cdots b_N \left\{ \Delta(\lambda) - \left(\rho + \frac{1}{\rho} \right) \right\}.$$

Of course the constant of integration $b_1 \cdots b_N \Delta(\lambda)$ is necessarily independent of ρ .

Let J be characterized by the data $\{u, y\}$. Then y_1, \dots, y_{N-1} are the first components of a set Y_1, \dots, Y_{N-1} of real, orthonormal eigenvectors of J corresponding to its eigenvalues u_1, \dots, u_{N-1} . Let $Y_{i,j}$ denote the i th component of Y_j . From the definition (6) of the Floquet multipliers and the identity (4) we infer that

$$\rho_j = - \frac{b_{N-1} Y_{N-1,j}}{b_N Y_{1,j}} \quad \forall j$$

and so

$$L_{\rho_j} \begin{bmatrix} Y_j \\ 0 \end{bmatrix} = \mu_j \begin{bmatrix} Y_j \\ 0 \end{bmatrix} \quad \forall j.$$

Consequently μ_j is an eigenvalue of L_{ρ_j} for each j and we infer from (7) that (8) is true.

From the definition (6) of the Floquet multipliers we deduce that

$$\omega'(\mu_j)\rho_j < 0 \quad \forall j.$$

When the eigenvalues of J are ordered so that

$$\mu_1 > \dots > \mu_{N-1}$$

then we infer from (8) that

$$(-1)^j \Delta(\mu_j) \geq 2 \quad \forall j$$

because the magnitude of $\rho + \frac{1}{\rho}$ is never less than two. Consequently the eigenvalues $\lambda_1, \dots, \lambda_N$ of L , which are the roots of $\Delta(\lambda) = 2$, are real and can be ordered so that

$$\lambda_1 > \lambda_2 > \lambda_3 > \lambda_4 > \lambda_5 > \dots$$

because the coefficient $(b_1 \dots b_N)^{-1}$ of λ^N in $\Delta(\lambda)$ is positive. ■

A typical discriminant for a periodic Jacobi matrix L of order $N = 6$ is illustrated in Figure 1. In this figure we depict the relationship between the eigenvalues $\lambda_1, \dots, \lambda_N$ of L and the Floquet multipliers $\rho_1, \dots, \rho_{N-1}$ of L corresponding to the eigenvalues μ_1, \dots, μ_{N-1} of J .

Let us introduce the following:

Definition 5: (a) The periodic Jacobi matrix L is characterized by the data $\{A, B, \mu, \rho\}$ if and only if

- (1) $A = a_1 + \dots + a_N$,
- (2) $B = b_1 \dots b_N$,
- (3) μ_1, \dots, μ_{N-1} are the eigenvalues of J , and
- (4) $\rho_1, \dots, \rho_{N-1}$ are the Floquet multipliers of L corresponding to μ_1, \dots, μ_{N-1} .

(b) The data $\{A, B, \mu, \rho\}$ is compatible if and only if

- (1) A is a real number,
- (2) B is a real, positive number,
- (3) μ_1, \dots, μ_{N-1} are real, distinct numbers, and
- (4) $\rho_1, \dots, \rho_{N-1}$ are real numbers which satisfy $\omega'(\mu_j)\rho_j < 0 \quad \forall j$ with $\omega(u) = (u - \mu_1) \dots (u - \mu_{N-1})$.

We feel justified in using the words "characterize" and "compatible" in this manner because the following theorem is true.

Theorem 6: Data characterizing a periodic Jacobi matrix is compatible. Furthermore, each set of compatible data $\{A, B, u, \rho\}$ characterizes a unique periodic Jacobi matrix L . The entries (a, b) of this periodic Jacobi matrix are computed by the algorithm:

1. $b_N^2 = - \sum_{k=1}^{N-1} \frac{B}{\rho_k \omega'(u_k)}$
2. $y_j = \frac{1}{b_N} \sqrt{- \frac{B}{\rho_j \omega'(u_j)}} \quad \forall j$
3. Recover J from the data $\{u, y\}$
4. $b_{N-1} = \frac{B}{b_1 \cdots b_{N-2} b_N}$
5. $a_N = A - (a_1 + \cdots + a_{N-1})$

with $\omega(u) = (u-u_1) \cdots (u-u_{N-1})$.

Proof: The proof of this theorem will be presented as a sequence of three lemmas.

Lemma 6.1: Data characterizing a periodic Jacobi matrix is compatible.

Proof: Let the periodic Jacobi matrix L be characterized by the data $\{A, B, u, \rho\}$. Clearly A is a real number because it is a sum of real numbers, while B is a real, positive number because it is a product of real, positive numbers. The u 's are real, distinct numbers because they are the eigenvalues of the Jacobi matrix J . While the definition (6) of the ρ 's makes it obvious that they are real, nonzero numbers which satisfy $\omega'(u_j) \rho_j < 0$ for all j because $\omega(u)$ is also the characteristic polynomial of J .

Lemma 6.2: Given compatible data $\{A, B, u, \rho\}$ the algorithm of Theorem 6 computes the entries (a, b) of a periodic Jacobi matrix L characterized by the data $\{A, B, u, \rho\}$.

Proof: The data $\{u, y\}$ used in step 3 is compatible, therefore it is clear that this algorithm computes the entries (a, b) of some periodic Jacobi matrix L . Let L be characterized by the data $\{\hat{A}, \hat{B}, \hat{u}, \hat{\rho}\}$. From steps 4 and 5 it is clear that $\hat{A} = A$ and $\hat{B} = B$. In view of Theorem 2 we know that J is characterized by the data $\{u, y\}$. Therefore $\hat{u}_j = u_j$ for all j and from the definition of the Floquet multipliers we know that

$$B = -\hat{\rho}_j \omega'(u_j) b_N^2 y_j^2 \quad \forall j.$$

Step 2 therefore implies that $\hat{\rho}_j = \rho_j$ for all j .

Lemma 6.3: Each set of compatible data characterizes at most one periodic Jacobi matrix.

Proof: Let \hat{L} be any periodic Jacobi matrix characterized by the compatible data $\{A, B, \mu, \rho\}$. Let the Jacobi matrix \hat{J} , obtained by deleting from \hat{L} the last row and column, be characterized by the data $\{\mu, \hat{y}\}$. Without loss of generality we may assume that each \hat{y}_j is positive, for if \hat{y}_j is the first component of an eigenvector \hat{Y}_j of \hat{J} then $-\hat{y}_j$ is the first component of the eigenvector $-\hat{Y}_j$ of \hat{J} . We will now prove that the entries (\hat{a}, \hat{b}) of \hat{L} are identical to the entries (a, b) of the periodic Jacobi matrix L constructed by the algorithm of Theorem 6.

By definition the Floquet multipliers $\hat{\rho}_1, \dots, \hat{\rho}_{N-1}$ of \hat{L} corresponding to μ_1, \dots, μ_{N-1} satisfy the relationship

$$B = -\rho_j \omega'(\mu_j) \hat{b}_N^2 \hat{y}_j^2 \quad \forall j.$$

The sum of the squares of the \hat{y} 's equals one because the data $\{\mu, \hat{y}\}$ is compatible, therefore

$$\hat{b}_N^2 = -\sum_{k=1}^{N-1} \frac{B}{\rho_k \omega'(\mu_k)} \quad \text{and} \quad \hat{y}_j = \frac{1}{\hat{b}_N} \sqrt{-\frac{B}{\rho_j \omega'(\mu_j)}} \quad \forall j.$$

In view of steps 1 and 2 we infer that $\hat{b}_N = b_N$ and $\hat{y}_j = y_j$ for all j . Since both \hat{J} and J are characterized by the same data then Theorem 2 implies that $\hat{J} = J$. Finally, steps 4 and 5 imply that $\hat{b}_{N-1} = b_{N-1}$ and $\hat{a}_N = a_N$.

4. Periodic Jacobi Matrices with Prescribed Spectra. With these basic facts established let us now consider how we can characterize the family of periodic Jacobi matrices whose eigenvalues are $\lambda_1, \dots, \lambda_N$.

Let L be a periodic Jacobi matrix characterized by the data $\{A, B, \mu, \rho\}$. Then $\lambda_1, \dots, \lambda_N$ are the eigenvalues of L if and only if the discriminant $\Delta(\lambda)$ of L admits the representation

$$\Delta(\lambda) = 2 + \frac{1}{B} (\lambda - \lambda_1) \cdots (\lambda - \lambda_N).$$

Therefore the problem of characterizing the family of periodic Jacobi matrices with prescribed spectra is intimately related to the problem of characterizing the family of periodic Jacobi matrices with prescribed discriminant. Let us introduce the following:

Definition 7: For each polynomial $p(\lambda)$ let $F(p)$ denote the family of periodic Jacobi matrices whose discriminant is $p(\lambda)$.

The problem of characterizing which periodic Jacobi matrices belong to $F(p)$ is answered in the following:

Theorem 8: Let $p(\lambda)$ be a polynomial of degree N . The data $\{A, B, u, \rho\}$ characterizes a member of $F(p)$ if and only if:

- (1) the data $\{A, B, u, \rho\}$ is compatible,
- (2) $p(\lambda) = \frac{1}{B} [\lambda^N - A \lambda^{N-1} + \text{lower powers of } \lambda]$, and
- (3) $p(u_j) = \rho_j + \frac{1}{\rho_j} \quad \forall j$.

Furthermore, $F(p)$ is nonempty if and only if

- (4) the coefficient of λ^N in $p(\lambda)$ is positive, and
- (5) $p(\lambda)$ has local extrema at $N-1$ real, distinct points $v_1 > \dots > v_{N-1}$ with $(-1)^j p(v_j) \geq 2 \quad \forall j$.

Proof: The proof of this theorem will be presented as a sequence of two lemmas. ■

Lemma 8.1: The data $\{A, B, u, \rho\}$ characterizes a member of $F(p)$ if and only if conditions (1,2,3) of Theorem 8 are satisfied.

Proof: If the data $\{A, B, u, \rho\}$ characterizes a member of $F(p)$ then Theorems 4 and 6 demonstrate that conditions (1,2,3) of Theorem 8 are satisfied.

Let us now suppose that conditions (1,2,3) of Theorem 8 are satisfied. Let $\Delta(\lambda)$ be the discriminant of the periodic Jacobi matrix characterized by the data $\{A, B, u, \rho\}$. Now

$$q(\lambda) \equiv \Delta(\lambda) - p(\lambda)$$

is a polynomial of degree $N-2$ because the coefficients of λ^{N-1} , λ^N in $\Delta(\lambda)$, $p(\lambda)$ agree. Theorem 4 also implies that $q(u_j) = 0 \quad \forall j$ and so

$$q(\lambda) \equiv 0$$

because the only polynomial of degree $N-2$ which is zero at $N-1$ distinct points is the trivial polynomial. Consequently the data $\{A, B, u, \rho\}$ characterizes a member of $F(p)$. ■

Lemma 8.2: $F(p)$ is nonempty if and only if conditions (4,5) of Theorem 8 are satisfied.

Proof: If $F(p)$ is nonempty then Lemma 8.1 and the mean-value theorem can be used to demonstrate that conditions (4,5) of Theorem 8 are satisfied.

Let us now suppose that conditions (4,5) of Theorem 8 are satisfied. Let A, B be determined so that

$$p(\lambda) = \frac{1}{B} [\lambda^N - A \lambda^{N-1} + \text{lower powers of } \lambda]$$

and $\rho_1, \dots, \rho_{N-1}$ be solutions of

$$p(v_j) = \rho_j + \frac{1}{\rho_j} \quad \forall j.$$

Then the data $\{A, B, v, \rho\}$ is compatible and from Lemma 8.1 we infer that the data $\{A, B, v, \rho\}$ characterizes a member of $F(p)$.

Using Theorem 8 it is not hard to prove the following:

Corollary 9: The periodic Jacobi matrix L has $\lambda_1, \dots, \lambda_N$ as its eigenvalues if and only if

$$L \in \bigcup_{B>0} F(\Lambda_B)$$

where $\Lambda_B(\lambda) \equiv 2 + \frac{1}{B}(\lambda - \lambda_1) \dots (\lambda - \lambda_N)$. Furthermore, there is a periodic Jacobi matrix with $\lambda_1, \dots, \lambda_N$ as its eigenvalues if and only if the numbers $\lambda_1, \dots, \lambda_N$ can be ordered so that

$$\lambda_1 > \lambda_2 > \lambda_3 > \lambda_4 > \lambda_5 > \dots$$

5. Numerical Experiments. Let us now present the results of several numerical experiments. These experiments were carried out on a UNIVAC 1110 in single precision floating point arithmetic (27 bit mantissa) using FORTRAN versions of the algorithms presented in Theorems 2 and 6.

In the first experiment we test the algorithm presented in Theorem 2. The results of this experiment are presented in Table 1. Observe that this algorithm has difficulty in recovering the Jacobi matrix described in Example 3.

Experiment 1:

1. Select a Jacobi matrix J of order $N-1$.
2. Compute the data $\{\mu, y\}$ characterizing J [13, 14, 15]:
 - (a) use bisection to compute the μ 's, and
 - (b) use inverse iteration to compute the y 's.
3. Use the algorithm presented in Theorem 2 to reconstruct the Jacobi matrix \hat{J} characterized by the data $\{\mu, y\}$.
4. Output the error $\|J - \hat{J}\|$ where

$$\|A\| = \max_{i,j} |a_{i,j}|.$$

In the second experiment we test the algorithm presented in Theorem 6. The results of this experiment are presented in Table 2. Observe that the Jacobi matrices used in the examples of Experiment 1 are obtained by deleting the last row and column from the periodic Jacobi matrix used in the corresponding examples of Experiment 2.

Experiment 2:

1. Select a periodic Jacobi matrix L of order N .
2. Compute the data $\{A, B, \mu, \rho\}$ characterizing L :
 - (a) use the obvious sum to compute A ,
 - (b) use the obvious product to compute B ,
 - (c) compute the data $\{\mu, y\}$ characterizing J as described in Step 2 of Experiment 1, and
 - (d) compute the ρ 's using Equation (6).
3. Use the algorithm presented in Theorem 6 to reconstruct the periodic Jacobi matrix \hat{L} characterized by the data $\{A, B, \mu, \rho\}$.
4. Output the error $\|L - \hat{L}\|$ where

$$\|A\| = \max_{i,j} |a_{ij}|.$$

In both of these experiments we have not worked with matrices of order $N > 30$. The reason why we have not worked with matrices of order $N > 30$ may be explained as follows. In Example 2 of Experiment 2 some of the components of y in the data $\{\mu, y\}$ become smaller as N increases. For example, the smallest component of y changes from 2×10^{-9} for $N = 15$ to 2×10^{-20} for $N = 30$. Since the Floquet multipliers ρ depend on the squares of the data y we will run into underflow problems when $N > 30$. The immediate remedy for this underflow problem is the use of logarithms in the computation of the Floquet multipliers. However, underflow also occurs in the computation of y when $N > 55$, consequently the use of logarithms is not a panacea.

6. Comments. Let $\tilde{\omega}(\mu)$ be the characteristic polynomial of the Jacobi matrix \tilde{J} obtained from J by deleting the first row and column. By comparing the entries of (2) in row 1, column 1 we find that

$$\tilde{\omega}(\mu) = \sum_{k=1}^{N-1} \frac{\omega(\mu)}{\mu - \mu_k} Y_{1,k}^2.$$

This identity was used by Stieltjes in his study of inverse eigenvalue problems. As μ tends to μ_j we deduce that

$$\tilde{\omega}(\mu_j) = \omega'(\mu_j) Y_{1,j}^2 \quad \forall j.$$

From this identity we infer that the eigenvalues of \tilde{J} strictly interlace those of J . Furthermore, from the eigenvalues of J and \tilde{J} we can recover the data $\{\mu, y\}$ characterizing J and hence J itself.

It is interesting to note that the algorithm presented in Theorem 2 is used in some versions of the implicit shift QR algorithm [13]. These versions of the QR algorithm make use of the fact that if $B = Q A Q^H$, where B is an unreduced upper Hessenberg matrix and Q is a unitary matrix, then the entries of B and Q are uniquely determined from the entries of A and the entries in the first row of Q . In our application $A = D$, $B = J$ and $Q = Y$.

We can also recover the Jacobi matrix J from the eigenvalues and the last components of the corresponding real, orthonormal eigenvectors of J . To understand why let us consider the permutation matrix

$$S = \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix}.$$

We find that $S^2 = I$, therefore from Equation (1) we deduce that

$$(SJS)(SY) = (SY)D.$$

Consequently the algorithm presented in Theorem 2 states that the entries of

$$SJS = \begin{bmatrix} a_{N-1} & b_{N-2} & 0 \\ b_{N-2} & & b_1 \\ 0 & b_1 & a_1 \end{bmatrix}$$

can be recovered from the entries of D and the entries in the first row of SY , that is the last row of Y .

It also appears that Theorem 2 can be extended to some class of band matrices. For example, let the real, symmetric matrix

$$K = \begin{bmatrix} a_1 & b_1 & c_1 & & 0 \\ b_1 & & & & \\ c_1 & & & & \\ & & & & \\ 0 & & c_{N-3} & b_{N-2} & a_{N-1} \end{bmatrix} \quad \text{where } c_i > 0 \quad \forall i.$$

have μ_1, \dots, μ_{N-1} as eigenvalues and Y_1, \dots, Y_{N-1} as the corresponding set of real, orthonormal eigenvectors. If Y denotes the matrix whose j th column is Y_j then Y is an orthogonal matrix and

$$KY = YD \quad \text{where} \quad D = \begin{bmatrix} \mu_1 & & 0 \\ & & \\ 0 & & \mu_{N-1} \end{bmatrix}.$$

Following the argument presented in Lemma 2.3 we arrive at an algorithm which recovers K from the entries in D and in the first two rows of Y .

The paper by Golub and Welsch [7] outlines how one can modify the usual QR algorithm and compute directly the data $\{\mu, \gamma\}$ characterizing a Jacobi matrix J . Furthermore, their paper also presents a matrix version of the celebrated Gelfand-Levitan solution to the inverse eigenvalue problem for a class of Sturm-Liouville problems.

The paper by Kammerer [10] describes an algorithm that can be used to construct a discriminant whose "shape" is prescribed. By the "shape" of a discriminant we are referring to the value of the discriminant at each of its $N-1$ real, distinct local extrema. For applications of Kammerer's algorithm to the periodic Toda lattice we refer the reader to the forthcoming paper [4].

Useful information concerning properties of periodic Jacobi matrices is contained in [1]. We would also like to state that the analysis presented in Section 3 can be extended in the same generality to "anti-periodic" Jacobi matrices of the form

$$L_{-1} = \begin{bmatrix} a_1 & b_1 & & & -b_N \\ & b_1 & & 0 & \\ & & & & b_{N-1} \\ & & 0 & & \\ -b_N & & & b_{N-1} & a_N \end{bmatrix} \quad \text{where } b_i > 0 \quad \forall i.$$

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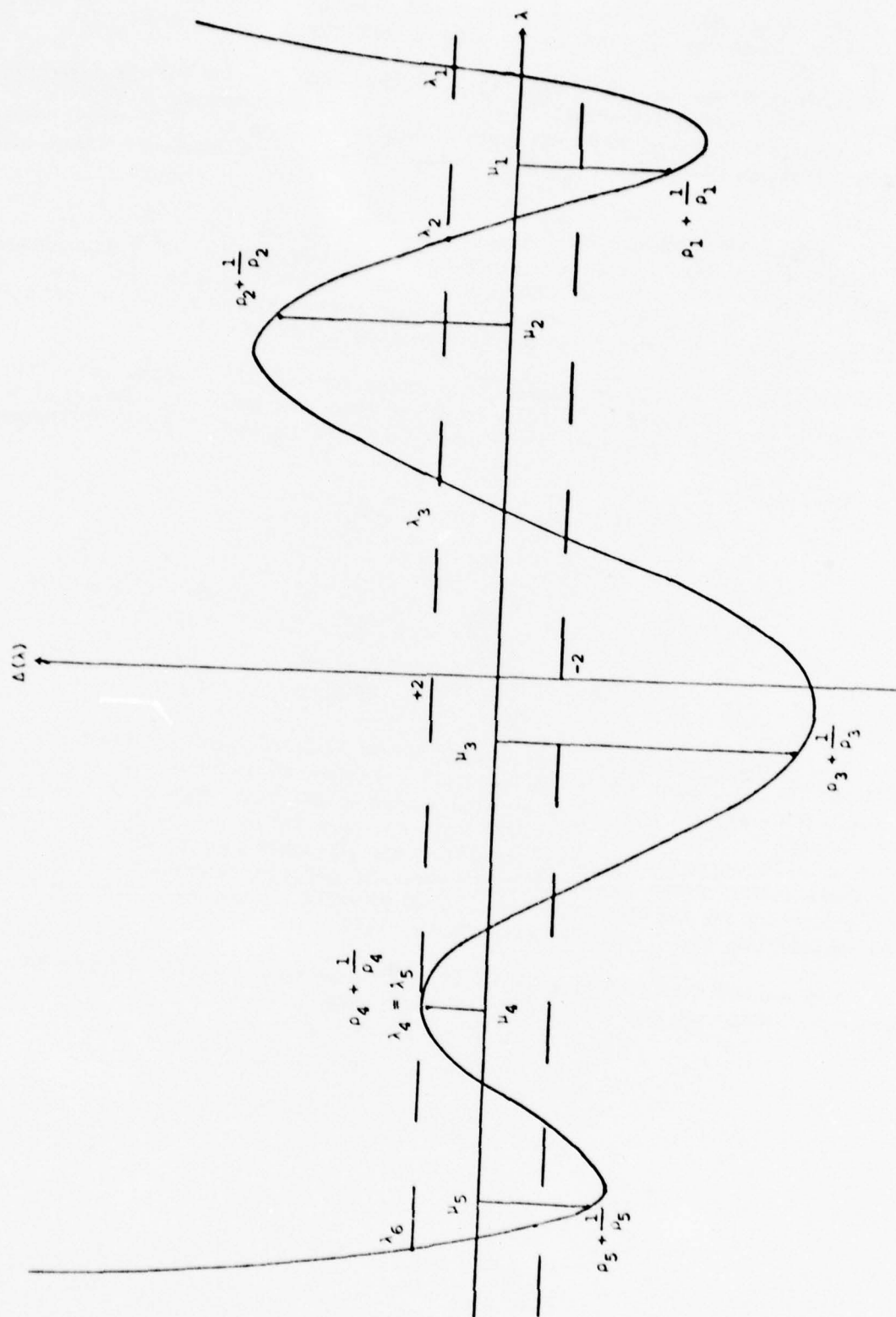


Figure 1: Plot of a Typical Discriminant, $N=6$

Example 1:

$$\begin{aligned} A(I) &= -2 & I &= 1, \dots, N-1 \\ B(I) &= 1 & I &= 1, \dots, N-2 \end{aligned}$$

N	Error
5	4×10^{-8}
10	2×10^{-7}
15	5×10^{-7}
20	2×10^{-7}
25	2×10^{-7}
30	6×10^{-7}

Example 2:

$$\begin{aligned} A(I) &= (N+1-I)/N-2 & I &= 1, \dots, N-1 \\ B(I) &= 1-(N-I)/N & I &= 1, \dots, N-2 \end{aligned}$$

N	Error
5	4×10^{-8}
10	1×10^{-7}
15	4×10^{-7}
20	3×10^{-7}
25	3×10^{-7}
30	9×10^{-7}

Table 1: Results of Experiment 1.

Example 3:

$$\begin{aligned} A(I) &= I/N - 2 & I &= 1, \dots, N-1 \\ B(I) &= 1 - I/N & I &= 1, \dots, N-2 \end{aligned}$$

N	Error
5	1×10^{-7}
10	3×10^{-7}
15	2×10^{-4}
20	2×10^0
25	2×10^0
30	1×10^0

Table 1: Results of Experiment 1.

Example 1:

$$\begin{aligned} A(I) &= -2 & I &= 1, \dots, N-1 \\ B(I) &= 1 & I &= 1, \dots, N-2 \\ A(N) &= 0 \\ B(N-1) &= B(N) = 1 \end{aligned}$$

N	Error
5	9×10^{-8}
10	5×10^{-7}
15	1×10^{-6}
20	2×10^{-6}
25	3×10^{-6}
30	5×10^{-6}

Example 2:

$$\begin{aligned} A(I) &= (N+1-I)/N-2 & I &= 1, \dots, N-1 \\ B(I) &= 1-(N-I)/N & I &= 1, \dots, N-2 \\ A(N) &= 0 \\ B(N-1) &= B(N) = 1 \end{aligned}$$

N	Error
5	1×10^{-7}
10	2×10^{-7}
15	4×10^{-7}
20	3×10^{-7}
25	6×10^{-7}
30	4×10^{-7}

Table 2 - Results of Experiment 2

Example 3:

$$A(I) = I/N-2 \quad I = 1, \dots, N-1$$

$$B(I) = 1 - I/N \quad I = 1, \dots, N-2$$

$$A(N) = 0$$

$$B(N-1) = B(N) = 1$$

N	Error
5	4×10^{-8}
10	1×10^{-7}
15	1×10^{-3}
20	2×10^0
25	4×10^0
30	5×10^0

Table 2. Results of Experiment 2.

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8. Appendix

In this section we present listings of several FORTRAN subroutines that the author used while performing various computational experiments.

No warranties, expressed or implied, are made by the author that this program is free of error. It should not be relied on as the sole basis to solve a problem whose incorrect solution could result in injury to person or property. If the program is employed in such a manner, it is at the user's own risk and the author disclaims all liability for such misuse.

```

===== DTAB =====
1.      SUBROUTINE DTAB(N,X,V,P)
2.      REAL X(N),V(N)
3.      COMMON /DIVTAB/ KDERV,NPTS,XNODE(51),DIVDF(51)
4.      C
5.      C      CONSTRUCT THE DIVIDED DIFFERENCE TABLE *NPTS,XNODE,DIVDF*
6.      C      BASED ON THE *N* NODES *X* AND THE CORRESPONDING FUNCTION
7.      C      VALUES *V*. THE DIVIDED DIFFERENCE TABLE IS CENTERED
8.      C      AT THE POINT *P*
9.      C
10.     C      INITIALIZE
11.     C
12.     NPTS = N
13.     DO 10 I=1,NPTS
14.         XNODE(I) = X(I)
15.         DIVDF(I) = V(I)
16.     10 CONTINUE
17.     C
18.     C      BUBBLE SORT THE NODES
19.     C
20.     DO 30 I=2,NPTS
21.         DO 20 K=2,I
22.             J = I-K+1
23.             IF (ABS(P-XNODE(J)).GE.ABS(P-XNODE(J+1))) GO TO 30
24.             EXCH = XNODE(J)
25.             XNODE(J) = XNODE(J+1)
26.             XNODE(J+1) = EXCH
27.             EXCH = DIVDF(J)
28.             DIVDF(J) = DIVDF(J+1)
29.             DIVDF(J+1) = EXCH
30.     20 CONTINUE
31.     30 CONTINUE
32.     C
33.     C      SET UP THE DIVIDED DIFFERENCE TABLE
34.     C
35.     DO 50 J=2,NPTS
36.         DO 40 K=J,NPTS
37.             I = K-J+1
38.             DIVDF(I) = (DIVDF(I+1)-DIVDF(I))/(XNODE(K)-XNODE(I))
39.         40 CONTINUE
40.     50 CONTINUE
41.     C
42.     RETURN
43.     C
44.     END

```

===== EIGEN =====

```

1.  SUBROUTINE EIGEN(N,A,B,MU,Y,D,W)
2.  REAL A(N),B(N),MU(N),Y(N),D(N),W(N),LO,HI,MID
3.  DATA NITS/10/
4.
5.  C      COMPUTE THE EIGNEVALUES *MU* AND THE FIRST COMPONENTS
6.  C      *Y* OF ORTHONORMAL EIGENVECTORS OF THE JACOBI MATRIX
7.  C
8.  C      A(1)  B(1)  0
9.  C      B(1)  :    :
10. C      :    :    :
11. C      :    :    :  R(N-1)
12. C      0    :    :  R(N-1)  A(N)
13. C
14. C      D,W ... WORKING STORAGE VECTORS OF LENGTH N .
15. C
16. C      NM1 = N-1
17. C
18. C      COMPUTE THE MACHINE EPSILON
19. C
20. C      EPS = 1.
21. 10 EPS = EPS/2.
22. C      TEST = 1.+EPS
23. C      IF (TEST.GT.1.) GO TO 10
24. C      EPS = 2.*EPS
25. C
26. C      COMPUTE GERSCHGORIN BOUNDS FOR THE EIGENVALUES
27. C
28. C      GMIN = A(1) - B(1)
29. C      GMAX = A(1) + B(1)
30. C      DO 20 I=2,NM1
31. C      GMIN = AMIN1(GMIN,A(I) - (B(I-1)+B(I)))
32. C      GMAX = AMAX1(GMAX,A(I) + (B(I-1)+B(I)))
33. 20 CONTINUE
34. C      GMIN = AMIN1(GMIN,A(N)-B(NM1))
35. C      GMAX = AMAX1(GMAX,A(N)+B(NM1))
36. C      SIZE = AMAX1(ABS(GMIN),ABS(GMAX))
37. C
38. C      COMPUTE *MU* AND *Y*
39. C
40. C      DO 120 I=1,N
41. C
42. C      COMPUTE *MU(I)* BY BISECTION
43. C
44. C      *NUM*, THE NUMBER OF NEGATIVE DIAGONAL ENTRIES IN
45. C      THE LU FACTORIZATION OF *MID - JACOBI*, COUNTS THE
46. C      NUMBER OF EIGENVALUES OF THE JACOBI MATRIX GREATER
47. C      THAN *MID*
48. C
49. C      LO = GMIN
50. C      HI = GMAX
51. 30 DIF = HI-LO
52. C      TEST = SIZE + DIF/2.
53. C      MID = LO + DIF/2.
54. C      IF (TEST.LE.SIZE) GO TO 50
55. C      TEST = EPS*SIZE
56. C      NUM = 0
57. C      O(1) = MID - A(1)

```

===== EIGEN =====

```

58.      IF (ABS(D(1)).LT.TEST) D(1) = SIGN(TEST,D(1))
59.      IF (D(1).LT.0.) NUM = NUM+1
60.      DO 40 J=2,N
61.          D(J) = (MID - A(J)) - R(J-1)**2/D(J-1)
62.          IF (ABS(D(J)).LT.TEST) D(J) = SIGN(TEST,D(J))
63.          IF (D(J).LT.0.) NUM = NUM+1
64.      40 CONTINUE
65.      IF (NUM.GE.1) LO = MID
66.      IF (NUM.LT.1) HI = MID
67.      GO TO 30
68.  C
69.  C      COMPUTE *Y(I)* BY INVERSE ITERATION
70.  C
71.  C      THE DIAGONAL ENTRIES OF THE LU FACTORIZATION OF
72.  C      *MID - JACOBI* HAVE BEEN COMPUTED ABOVE
73.  C
74.      50 W(1) = 1.
75.      DO 60 J=2,N
76.          W(J) = 0.
77.      60 CONTINUE
78.      DO 110 IT=1,NITS
79.          DO 70 J=1,NM1
80.              W(J+1) = W(J+1) + B(J)*W(J)/D(J)
81.      70 CONTINUE
82.          W(N) = W(N)/D(N)
83.          DO 80 JR=1,NM1
84.              J = N-JR
85.              W(J) = (W(J) + B(J)*W(J+1))/D(J)
86.      80 CONTINUE
87.          SUM = 0.
88.          DO 90 J=1,N
89.              SUM = SUM + W(J)**2
90.      90 CONTINUE
91.          SUM = SQRT(SUM)
92.          DO 100 J=1,N
93.              W(J) = W(J)/SUM
94.      100 CONTINUE
95.      110 CONTINUE
96.  C
97.      MU(I) = MID
98.      Y(I) = W(1)
99.  C
100.      120 CONTINUE
101.  C
102.      RETURN
103.  C
104.      END

```


===== FALST =====

```

1.  FUNCTION FALST(A,R,TOL,F,VALUE,IFLAG)
2.  C
3.  C      IN THE INTERVAL BETWEEN *A* AND *R* COMPUTE TO AN ACCURACY
4.  C      *TOL* THE LOCATION *FALST* WHERE *F* ASSUMES *VALUE*.
5.  C      IF UPON RETURN
6.  C
7.  C      IFLAG = 1 ... THEN *FALST* WAS FOUND TO AN ACCURACY OF *TOL*
8.  C      2 ... THEN *TOL* WAS NEGATIVE
9.  C      3 ... THEN F(X)=VALUE HAS THE SAME SIGN AT X=A,R
10. C
11. C      IF *TOL* IS ZERO THEN *FALST* IS FOUND TO MACHINE PRECISION
12. C
13. C      IFLAG = 1
14. C
15. C      CHECK LEFT ENDPOINT FOR A ZERO
16. C
17. C      FALST = AMIN(A,R)
18. C      F1 = F(FALST) - VALUE
19. C      IF (F1.EQ.0.) RETURN
20. C      X1 = FALST
21. C      TEST = F1
22. C
23. C      CHECK RIGHT ENDPOINT FOR A ZERO
24. C
25. C      FALST = AMAX(A,R)
26. C      F2 = F(FALST) - VALUE
27. C      IF (F2.EQ.0.) RETURN
28. C      X2 = FALST
29. C
30. C      CHECK FOR REASONABLE *TOL*
31. C
32. C      IF (TOL.GE.0.) GO TO 10
33. C      IFLAG = 2
34. C      RETURN
35. C
36. C      CHECK FOR SIGN CHANGE
37. C
38. C      10 IF (F1*SIGN(1.,F2).LT.0.) GO TO 20
39. C      IFLAG = 3
40. C      RETURN
41. C
42. C      LINEAR INTERPOLATION USED TO COMPUTE APPROXIMATE LOCATION
43. C      OF THE ZERO
44. C
45. C      20 SAVE = TEST
46. C      RATIO = F1/(F1-F2)
47. C      FALST = X1 + RATIO*(X2-X1)
48. C
49. C      CHECK FOR TERMINATION
50. C
51. C      IF ( (X2-X1).LE.TOL*AMAX(ABS(X1),ABS(X2)) ) RETURN
52. C
53. C      CHECK IF GUESS FOR ZERO IS ACCEPTABLE
54. C
55. C      IF ( (FALST.GT.X1).AND.(FALST.LT.X2) ) GO TO 30
56. C
57. C      IF THE MIDDPOINT IS ALSO UNACCEPTABLE THEN *TOL* IS TOO SMALL

```

```

      ===== FALST =====
58.      C      AND *FALST* IS THE BEST THAT CAN BE DONE
59.      C
60.      FALST = X1 + .5*(X2-X1)
61.      IF ( (FALST.LE.X1).OR.(FALST.GE.X2) ) RETURN
62.      C
63.      C      UPDATE INFORMATION
64.      C
65.      30 TEST = F(FALST) - VALUE
66.      IF (TEST*SIGN(1.,F1)) 40,50,60
67.      C
68.      40 X2 = FALST
69.      F2 = TEST
70.      IF (TEST*SIGN(1.,SAVE).GT.0.) F1 = .5*F1
71.      GO TO 20
72.      C
73.      50 RETURN
74.      C
75.      60 X1 = FALST
76.      F1 = TEST
77.      IF (TEST*SIGN(1.,SAVE).GT.0.) F2 = .5*F2
78.      GO TO 20
79.      C
80.      END

```

===== JACOB =====

```

1.  SUBROUTINE JACOB(N,A,R,MU,Y,W1,W2)
2.  REAL A(N),R(N),MU(N),Y(N),W1(N),W2(N)
3.
4.  C      CONSTRUCT THE ENTRIES (A,R) OF A JACOBI MATRIX
5.  C
6.  C      A(1)    R(1)                                0
7.  C      R(1)    .      .
8.  C      .      .      .      .
9.  C      .      .      .      .      R(N-1)
10. C      0      .      .      .      R(N-1)  A(N)
11. C
12. C      WHERE Y(J) IS THE FIRST COMPONENT OF A NORMALIZED
13. C      EIGENVECTOR OF THE JACOBI MATRIX CORRESPONDING TO THE
14. C      EIGENVALUE MU(J) .
15. C
16. C      WE ASSUME THAT THE MUIS ARE REAL,DISTINCT NUMBERS AND
17. C      THE Y'S ARE REAL, NONZERO NUMBERS WHOSE SQUARES SUM TO
18. C      ONE.
19. C
20. C      W1,W2 ... WORKING STORAGE VECTORS OF LENGTH N .
21. C
22. C      IF THE USER DOES NOT NEED Y TO BE SAVED THEN CALL THIS
23. C      PROGRAM WITH THE W1 ARGUMENT EQUAL TO Y .
24. C
25. C      NM1 = N-1
26. C
27. C      INITIALIZE
28. C
29. C      DO 10 I=1,N
30. C        W1(I) = Y(I)
31. C        W2(I) = 0.
32. C      10 CONTINUE
33. C
34. C      RIM1 = 0.
35. C      DO 50 I=1,NM1
36. C
37. C        COMPUTE *A(I)*
38. C
39. C        A(I) = 0.
40. C        DO 20 K=1,N
41. C          A(I) = A(I) + MU(K)*W1(K)**2
42. C      20 CONTINUE
43. C
44. C        COMPUTE *B(I)*
45. C
46. C        R(I) = 0.
47. C        DO 30 K=1,N
48. C          T = (MU(K)-A(I))*W1(K) - RIM1*W2(K)
49. C          R(I) = R(I) + T**2
50. C      30 CONTINUE
51. C        R(I) = SQRT(R(I))
52. C
53. C        COMPUTE THE NEXT *Y*
54. C
55. C        DO 40 K=1,N
56. C          T = (MU(K)-A(I))*W1(K) - RIM1*W2(K)
57. C          W2(K) = W1(K)

```

===== JACOB =====

```

58.      W1(K) = T/R(I)
59.      40 CONTINUE
60.      C
61.      RIM1 = R(I)
62.      50 CONTINUE
63.      C
64.      C      COMPUTE *A(N)*
65.      C
66.      A(N) = 0.
67.      DO 60 K=1,N
68.      A(N) = A(N) + MU(K)*W1(K)**2
69.      60 CONTINUE
70.      C
71.      RETURN
72.      C
73.      END

```


===== KAMMER =====

```

1. SUBROUTINE KAMMER(NP1,X,V,W1,IFLAG)
2. REAL X(NP1),V(NP1),W1(NP1)
3. COMMON /DIVTR/ KDERV,NPTS,XNODE(51),DIVDF(51)
4. DATA PI/3.14159265358/
5. EXTERNAL POLYV
6.
7. C
8. C      GIVEN OSCILLATING DATA *V* COMPUTE THE NODES *X* OF
9. C      THE UNIQUE INTERPOLATING POLYNOMIAL *P(X)* FOR WHICH
10. C
11. C      1)  $0 \leq X(NP1) \leq 1$  ...  $0 \leq X(1) \leq 1$ 
12. C      2)  $P(X(I)) = V(I)$  FOR  $I=1, \dots, NP1$ 
13. C      3)  $DP(X(I))/DX = 0$  FOR  $I=2, \dots, NP1-1$ 
14. C
15. C      IF UPON RETURN
16. C
17. C      IFLAG = 1 ... THEN EVERYTHING WORKED
18. C      2 ... THEN THE DATA *V* DOES NOT OSCILLATE .
19. C
20. C      W1 ... WORKING STORAGE VECTOR OF LENGTH NP1 .
21. C
22. C      N = NP1-1
23. C
24. C      CHECK THAT THE DATA *V* OSCILLATES
25. C
26. C      IFLAG = 2
27. C      DP = V(2) - V(1)
28. C      IF (DP.EQ.0.) RETURN
29. C      DO 10 I=2,N
30. C      DP = V(I+1) - V(I)
31. C      IF (DP*SIGN(1.,DP).GE.0.) RETURN
32. C      10 CONTINUE
33. C
34. C      INITIALIZE
35. C
36. C      IFLAG = 1
37. C      X(1) = 1.
38. C      DO 20 I=2,N
39. C      X(I) = .5*(1.+COS((I-1)*PI/N))
40. C      20 CONTINUE
41. C      X(NP1) = 0.
42. C      CALL DTARL(NP1,X,V,0.)
43. C
44. C      COMPUTE THE MID-V POINTS
45. C
46. C      30 SAVE = DIVDF(1)
47. C      KDERV = 0
48. C      DO 40 I=1,N
49. C      XMID = X(I) + .5*(X(I+1)-X(I))
50. C      CALL DTARL(NP1,X,V,XMID)
51. C      VMID = V(I) + .5*(V(I+1)-V(I))
52. C      X(I) = FALST(X(I),X(I+1),0.,POLYV,VMID,IFLAG)
53. C      40 CONTINUE
54. C
55. C      COMPUTE THE ZEROS OF THE DERIVATIVE
56. C
57. C      KDERV = 1

```


***** KAMMER *****

```

58.      DO 50 I=2,N
59.          CALL DTABL(NP1,X,V,X(I))
60.          W1(I-1) = FALST(W1(I-1),W1(I),0.,POLYV,0.,TERR)
61.      50 CONTINUE
62.      C
63.      C      UPDATE THE NODES
64.      C
65.      DO 60 I=2,N
66.          X(I) = W1(I-1)
67.      60 CONTINUE
68.      C
69.      C      TEST FOR COMPLETION
70.      C
71.      CALL DTABL(NP1,X,V,0.)
72.      IF (ABS(SAVE).LE.ABS(DIVDE(1))) RETURN
73.      GO TO 30
74.      C
75.      END

```

===== PEIGEN =====

SUBROUTINE PEIGEN(N,A,R,MU,RHO,W1,W2)
REAL A(N),R(N),MU(N),RHO(N),W1(N),W2(N)

COMPUTE THE EIGENVALUES *MU* OF THE LEADING PRINCIPLE
SUBMATRIX OF THE PERIODIC JACOBI MATRIX

```

      A(1)  R(1)                                R(N)
      R(1)  .      .      .      .
      .      .      .      .
      .      .      .      .
      R(N)  0      .      .      R(N-1)
                                R(N-1)  A(N)

```

AND THEIR CORRESPONDING FLOQUET MULTIPLIERS *RHO*. THE
SUM OF THE A'S IS STORED IN MU(N) AND THE PRODUCT
OF THE R'S IS STORED IN RHO(N).

W1,W2 ... WORKING STORAGE VECTORS OF LENGTH N.

NM1 = N-1

COMPUTE MU(N) AND RHO(N)

MU(N) = 0.

RHO(N) = 1.

DO 10 I=1,N

MU(N) = MU(N) + A(I)

RHO(N) = RHO(N)*R(I)

10 CONTINUE

COMPUTE THE EIGENVALUES *MU* AND THE FIRST COMPONENTS
RHO OF ORTHONORMAL EIGENVECTORS OF THE LEADING
PRINCIPLE SUBMATRIX

CALL EIGEN(NM1,A,R,MU,RHO,W1,W2)

REPLACE *RHO* BY THE FLOQUET MULTIPLIERS CORRESPONDING TO
THE EIGENVALUES *MU*.

DO 30 I=1,NM1

PROD = 1.

DO 20 J=1,NM1

IF (I.NE.J) PROD = PROD*(MU(I)-MU(J))

20 CONTINUE

RHO(I) = -RHO(N)/(PROD*(R(N)+RHO(I)+*2)

30 CONTINUE

RETURN

END

===== PJACOB =====

SUBROUTINE PJACOB(N,A,B,MU,RHO,W1,W2)
REAL A(N),R(N),MU(N),RHO(N),W1(N),W2(N)

CONSTRUCT THE ENTRIES (A,B) OF A PERIODIC JACOBI MATRIX

A(1)	R(1)			R(N)
R(1)	.	.	0	
	.	.	.	R(N-1)
R(N)	0	.	R(N-1)	A(N)

WHERE RHO(J) IS THE FLOQUET MULTIPLIER CORRESPONDING TO THE EIGENVALUE MU(J) OF THE LEADING PRINCIPLE SUBMATRIX. THE SUM OF THE A'S IS STORED IN MU(N) AND THE PRODUCT OF THE R'S IS STORED IN RHO(N).

WE ASSUME THAT THE SUM OF THE A'S IS REAL, THE PRODUCT OF THE R'S IS REAL AND POSITIVE, THE MU'S ARE REAL AND DISTINCT, AND THE RHO'S ARE REAL AND NONZERO NUMBERS WHICH SATISFY

$\Omega(\mu(j)) = \mu(j) + RHO(j) \cdot LT. 0.$
FOR ALL J WHERE
 $\Omega(x) = (x - \mu(1)) \cdot \dots \cdot (x - \mu(N-1))$

W1,W2 ... WORKING STORAGE VECTORS OF LENGTH N.

IF THE USER DOES NOT NEED RHO TO BE SAVED THEN CALL THIS PROGRAM WITH THE W1 ARGUMENT EQUAL TO RHO.

NM1 = N-1
NM2 = N-2

RECOVER *R(N)*

```

DO 10 I=1,NM2
  W2(I) = MU(I+1)
10 CONTINUE
R(N) = 0.
DO 30 K=1,NM1
  DERV = 1.
  DO 20 I=1,NM2
    DERV = DERV*(MU(K)-W2(I))
  20 CONTINUE
  R(N) = R(N) + RHO(N)/(RHO(K)*DERV)
  W2(K) = MU(K)
30 CONTINUE
R(N) = SQRT(R(N))

```

RECOVER THE FIRST COMPONENTS *W1* OF THE ORTHONORMAL EIGENVECTORS OF THE LEADING PRINCIPLE SUBMATRIX.

```

DO 40 I=1,NM2
  W2(I) = MU(I+1)
40 CONTINUE
DO 60 K=1,NM1
  DERV = 1.

```

```

===== PJACOR =====
58.      DO 50 I=1,NM2
59.      DERV = DERV+(MU(K)-W2(I))
60.      50 CONTINUE
61.      W1(K) = SQRT(-RHO(N)/(RHO(K)+DERV))/R(N)
62.      W2(K) = MU(K)
63.      60 CONTINUE
64.      C
65.      C      RECOVER THE LEADING PRINCIPLE SUBMATRIX
66.      C
67.      CALL JACOR(NM1,4,R,MU,W1,W1,W2)
68.      C
69.      C      RECOVER *R(N-1)*
70.      C
71.      R(NM1) = RHO(N)/R(N)
72.      DO 70 K=1,NM2
73.      R(NM1) = R(NM1)/R(K)
74.      70 CONTINUE
75.      C
76.      C      RECOVER *A(N)*
77.      C
78.      A(N) = MU(N) - A(NM1)
79.      DO 80 K=1,NM2
80.      A(N) = A(N) - A(K)
81.      80 CONTINUE
82.      C
83.      RETURN
84.      C
85.      END

```

```

===== POLYV =====
1.      FUNCTION POLYV(X)
2.      COMMON /DIVTR/ KDERV,NPTS,XNODE(S1),DIVDF(S1)
3.      C
4.      C      COMPUTE THE VALUE *POLYV* OF THE INTERPOLATING POLYNOMIAL
5.      C      *KDERV=0* OR ITS DERIVATIVE *KDERV=1* AT *X* BASED ON THE
6.      C      DESCRIPTION GIVEN IN THE DIVIDED DIFFERENCE TABLE
7.      C      *NPTS,XNODE,DIVDF*
8.      C
9.      C      HORNER'S ALGORITHM IS USED TO COMPUTE THE VALUE REQUIRED.
10.     C
11.     POLY = 0.
12.     DPOLY = 0.
13.     DO 10 I=1,NPTS
14.     DPOLY = POLY + (X-XNODE(I))*DPOLY
15.     POLY = DIVDF(I) + (X-XNODE(I))*POLY
16.     10 CONTINUE
17.     C
18.     POLYV = POLY
19.     IF (KDERV.EQ.1) POLYV = DPOLY
20.     C
21.     RETURN
22.     C
23.     END

```



```

      ===== RSCALE =====
1.      SUBROUTINE RSCALE(NP1,X,V)
2.      REAL X(NP1),V(NP1)
3.      COMMON /DIVTR/ KDERV,NPTS,XNODE(51),DIVDF(51)
4.      C
5.      C      SCALE THE DATA *X,V* SO THE DISCRIMINANT IT DESCRIBES
6.      C      CHARACTERIZES A PERIODIC JACOBI MATRIX WHOSE SUM OF THE
7.      C      A'S IS ZERO AND WHOSE PRODUCT OF THE B'S IS  $2^{*}(-N)$  .
8.      C
9.      N = NP1-1
10.     SUM = 0.
11.     DO 10 I=2,NP1
12.       SUM = SUM + X(I)
13.     10 CONTINUE
14.     C
15.     CALL DTARL(NP1,X,V,X(NP1))
16.     SHIFT = (DIVDF(2)-SUM*DIVDF(1))/(N*DIVDF(1))
17.     EXPAN = EXP(-(N*ALOG(2.)-ALOG(DIVDF(1)))/N)
18.     DO 20 I=1,NP1
19.       X(I) = EXPAN*(X(I)+SHIFT)
20.     20 CONTINUE
21.     C
22.     RETURN
23.     END

```

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